

Unconventional Hall effect in pnictides from interband interactions

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We calculate the Hall transport in a multiband systems with a dominant interband interaction between carriers having electron and hole character. We show that this situation gives rise to an unconventional scenario, beyond the Boltzmann theory, where the quasiparticle currents dressed by vertex corrections acquire the character of the majority carriers. This leads to a larger (positive or negative) Hall coefficient than what expected on the basis of the carrier balance, with a marked temperature dependence. Our results explain the puzzling measurements in pnictides and they provide a more general framework for transport properties in multiband materials.

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The discovery of superconductivity in iron-based superconductors has triggered a renewed interest in the properties of interacting multiband systems. Indeed, all the families of pnictides display several hole (h) and electron (e) pockets at the Fermi level, as predicted by density-functional-theory calculations and confirmed by Fermi-surface sensitive experiments, as de Haas van Alphen and photoemission spectroscopy[1]. A much more indirect probe of such a multiband character comes from transport experiments, where the contribution of carriers having h and e character is unavoidably mixed. A typical example is provided by Hall-effect measurements, for which a standard Boltzmann-like multicarrier picture[2] would give a Hall coefficient

$$R_H^0 = \frac{1}{e} \frac{(n_h \mu_h^2 - n_e \mu_e^2)}{(n_h \mu_h + n_e \mu_e)^2}, \quad (1)$$

where n_α ($\alpha = e, h$) is the density of the e- or h- carrier type, and $\mu_\alpha = e^2 \tau_\alpha / m_\alpha$ the corresponding mobility, with τ_α being the transport scattering time and m_α the effective carrier mass in each band. In compensated semimetals as pnictides, where $n_e \approx n_h$, one would thus expect an almost vanishing Hall coefficient. Striking enough, most pnictides [3–9] show a quite different scenario with a very large absolute value of the Hall coefficient R_H , and with a marked e/h character of the transport in materials which are only slightly e/h doped. In addition, a strong temperature dependence of R_H is also typically found, that disappears only at very large doping away from half-filling. Since $\mu_\alpha \propto \tau_\alpha$, to account for these features within the Boltzmann-like approach (1) one needs thus to assume a marked disparity between τ_e and τ_h , with $\tau_e \gg \tau_h$ in e-doped compounds and $\tau_h \gg \tau_e$ in the h-doped ones. However, such a disparity has not been supported until now by any explicit calculation. For example, the inclusion of spin[10] or orbital[11] fluctuations within realistic models can account at most for a factor of 2 of anisotropy between the average quasiparticle lifetime on the e and h pockets, not enough to explain

neither the absolute value of R_H nor its T dependence reported in Refs. [3–9]. In addition, the claim of two very different scattering rates in pnictides obtained from optical probes, where the flat mid-infrared optical conductivity is sometimes attributed to a very broad Drude-like intraband contribution [12–14], has been questioned by several authors on the basis of the presence in pnictides of low-energy interband optical transitions [13, 15–17]. A convincing framework to explain the unconventional properties of the Hall transport in pnictides, and hence to elucidate the role of the scattering mechanisms, is thus still lacking in these materials.

In this Letter we show that in a multiband system with predominant interband interactions between carriers having opposite (e/h) character the semiclassical picture of transport based on Eq. (1) must be strongly revised. By computing explicitly the current vertex corrections due to the exchange of spin fluctuations between h and e bands, we show that, in contrast to the standard Fermi-liquid case, they cannot be simply recast in a renormalization of the transport scattering time with respect to the quasiparticle lifetime. Indeed, the spin fluctuations induce a mixing of the electron and hole currents such that the renormalized current in each band can even have opposite direction with respect to the bare band velocity. This mechanism explains the large value of $|R_H|$ in slightly e/h doped compounds, and its temperature and doping dependence, in good agreement with the experimental findings in the non-magnetic state.

Let us introduce the minimal model which contains the main ingredients responsible for the unconventional Hall transport in pnictides. We consider a two-band model with two-dimensional parabolic e/h bands centered at the Γ and $M = \mathbf{Q} = (\pi, \pi)$ points, with different Fermi-surface (FS) areas:

$$\xi_{\mathbf{k}}^h = E_{max}^h - \frac{\mathbf{k}^2}{2m_e} - \mu, \quad \xi_{\mathbf{k}}^e = -E_{min}^e + \frac{\mathbf{k}^2}{2m_h} - \mu, \quad (2)$$

where \mathbf{k} is the reduced momentum with respect to the Γ

or M point, for the h or e band, respectively. We take here units $\hbar = c = a = 1$ (a being the lattice spacing). In the following we choose $\mu = 0$, so that E_{min}^e and E_{max}^h fix the Fermi wavevectors $k_F^{e,h}$ in each band, and we will assume, without loss of generality, $m_e = m_h = m$. The general gauge-invariant expression for the longitudinal and transverse conductivities for each band $\alpha=e,h$ can be derived on the basis of the Kubo formula for a weakly interacting system [18, 19]. In particular we have that

$$\sigma_{xx}^\alpha = e^2 \sum_{\mathbf{k}} \left(-\frac{\partial f}{\partial \xi} \right)_{\xi_{\mathbf{k}}} v_x^\alpha(\mathbf{k}) J_x^\alpha(\mathbf{k}) \frac{1}{\Gamma^\alpha(\mathbf{k})} \simeq \frac{e^2}{2} \frac{\mathbf{J}_F^\alpha \cdot \mathbf{k}_F^\alpha}{2\pi \Gamma_F^\alpha}, \quad (3)$$

where the derivative of the Fermi function $f(x) = (1 + e^{x/T})^{-1}$ has been approximated at low temperature T with a δ -function, so that only quantities at the FS appear in the final expression. In Eq. (3) the vector \mathbf{v}^α denotes the band velocity in the x - y plane for the band α , \mathbf{J}^α is the corresponding renormalized current and Γ^α is the inverse quasiparticle lifetime, determined in general by electron-electron and impurity scattering processes. Due to the symmetry of the problem, \mathbf{J}^α is parallel to the reduced momentum \mathbf{k} in each band α , and $\Gamma^\alpha(\mathbf{k})$ and $\mathbf{J}^\alpha(\mathbf{k})$ depend only on $|\mathbf{k}|$, so we define their value at the FS as $\Gamma_F^\alpha \equiv \Gamma^\alpha(k_F^\alpha)$ and $\mathbf{J}_F^\alpha \equiv \mathbf{J}^\alpha(k_F^\alpha)$. The transverse xy conductivity under a weak magnetic field H along the z axis can be written as:

$$\frac{\sigma_{xy}}{H} = -\frac{e^3}{4} \sum_{\mathbf{k}} \left(-\frac{\partial f}{\partial \xi} \right)_{\xi_{\mathbf{k}}} \frac{A^\alpha(\mathbf{k})}{(\Gamma^\alpha(\mathbf{k}))^2} \simeq \mp \frac{e^3}{8\pi} \frac{(J_F^\alpha)^2}{(\Gamma_F^\alpha)^2}, \quad (4)$$

where $A^\alpha(\mathbf{k}) = v^\alpha [\mathbf{J}^\alpha \times (\mathbf{e}_\parallel^\alpha \cdot \nabla) \mathbf{J}^\alpha] \cdot \mathbf{e}_z$. Here \mathbf{e}_z is the unit vector along the z axis, while $\mathbf{e}_\parallel^\alpha = (\mathbf{e}_z \times \mathbf{v}^\alpha)/|\mathbf{v}^\alpha|$ is tangential to the α -th FS at \mathbf{k} . For a parabolic band we have thus $\mathbf{e}_\parallel^\alpha \cdot \nabla = \pm \partial_\theta/k$, where the plus/minus sign holds for an e/h band, respectively, so that $A^\alpha = \pm(v^\alpha/k)(\mathbf{J}^\alpha \times \partial_\theta \mathbf{J}^\alpha)_z = \pm v^\alpha (J^\alpha)^2/k$. As a consequence, the overall sign in Eq. (4) is determined only by the sign of $\mathbf{v} \cdot \mathbf{k}$, which identifies the e/h character of the band[20]. Once evaluated the longitudinal and transverse conductivity, the Hall coefficient R_H is given by

$$R_H = \frac{\sum_i \sigma_{xy}^i}{(\sum_i \sigma_{xx}^i)^2 H_z}. \quad (5)$$

Eqs. (3)-(5) are quite general, since they express the conductivities in terms of the bare Fermi velocity \mathbf{v}^α and the renormalized current \mathbf{J}^α . What makes multiband systems peculiar is the nature of vertex corrections that determine the relation between \mathbf{v}^α and \mathbf{J}^α . Using a standard approach[21] one can establish between these two quantities a matricial relation

$$\mathbf{J}_F^\alpha = \Lambda_{\alpha\beta} \mathbf{v}_F^\beta. \quad (6)$$

The case $\Lambda_{\alpha\beta} = \delta_{\alpha\beta}$ corresponds to the non-interacting system where, by using the 2D relation $n_\alpha = (\mathbf{k}_F^\alpha)^2/2\pi$

and by identifying $1/\tau_\alpha = 2\Gamma_F^\alpha$, Eqs. (3)-(4) reduce to the standard results, $\sigma_{xx}^\alpha = e^2 n_\alpha \tau_\alpha / m$ and $\sigma_{xy}^\alpha = \mp \sigma_{xx}^\alpha \mu_\alpha H$, with $\mu_\alpha = e\tau_\alpha/m$, and the minus/plus sign holds for the e/h band, respectively. In the interacting case, the strength of the diagonal and off-diagonal coefficients $\Lambda_{\alpha\beta}$ depends on the intraband or interband interactions, respectively. In conventional materials with predominance of intraband scattering $\mathbf{J}_F^\alpha = \Lambda_{\alpha\alpha} \mathbf{v}_F^\alpha$, so that the effect of vertex corrections in Eq.(3) and (4) can be reabsorbed in the definition of the transport scattering time $\tau_\alpha = \Lambda_{\alpha\alpha}/2\Gamma_F^\alpha$, and the result (1) still holds, with renormalized mobilities. Things are however deeply different in multiband systems with dominant interband interactions connecting e and h sheets, as in pnictides. In this case the largest elements in $\Lambda_{\alpha\beta}$ are off-diagonal, leading to a mixing of the e and h characters and resulting in unconventional features, like a possible vanishing current \mathbf{J}_F^α . In this situation, although the conductivities are still diagonal in the band index α (as one can show following the general derivation of Ref. [19]), Eq. (5) cannot be reduced to the Boltzmann-like result (1).

To investigate in details this issue, in the following we compute explicitly both Γ_F^α and \mathbf{J}_F^α in the representative case of pnictides, where the carriers in the h and e bands interact via spin-fluctuations (SF) exchange[1]. According to neutron-scattering experiments[22], the SF spectrum can be phenomenologically modeled with a standard marginal-Fermi-liquid spectrum,

$$\chi(\mathbf{q} - \mathbf{Q}, \omega) = \frac{\chi_Q}{1 + \xi_T^2(\mathbf{q} - \mathbf{Q})^2 + i\omega/\omega_{sf}}, \quad (7)$$

where $\chi_Q = \chi_0 \Theta / (T + \Theta)$ is the strength of the SF, $\omega_{sf} = \omega_0(T + \Theta)/\Theta$ is their frequency scale and $\xi_T = \xi_0 \sqrt{\Theta/(T + \Theta)}$ is the AF correlation length, with Θ Curie-Weiss temperature. Since the SF are peaked around the $\Gamma - M$ nesting vector $\mathbf{q} = \mathbf{Q}$, the interaction mediated by such a collective mode will have a predominant interband character. The crucial role of such interband retarded interaction has been already demonstrated for the understanding of several spectroscopic[23–25], thermodynamic[24, 26] and optical[27] anomalies of pnictides. However, to compute current vertex corrections the explicit momentum dependent of the bosonic spin spectrum (7), neglected so far in Refs. [23–27], must be taken into account. For the sake of simplicity we assume in the following that only interband scattering is present, neglecting any intraband coupling. The single-particle Green's function in each band is computed as usual by means of the Dyson equation $G^{\alpha-1}(\mathbf{k}, i\omega_n) = i\omega_n - \xi_{\mathbf{k}}^\alpha - \Sigma^\alpha(\mathbf{k}, i\omega_n)$, where the self-energy is given by

$$\Sigma^\alpha(\mathbf{k}, \omega_n) = g^2 T \sum_{\mathbf{q}, l} \chi(\mathbf{q}, i\omega_l) G^\beta(\mathbf{k} - \mathbf{q}, \omega_n - \omega_l), \quad (8)$$

where ω_n, ω_l are fermionic and bosonic Matsubara frequencies, respectively, and g is the coupling to the

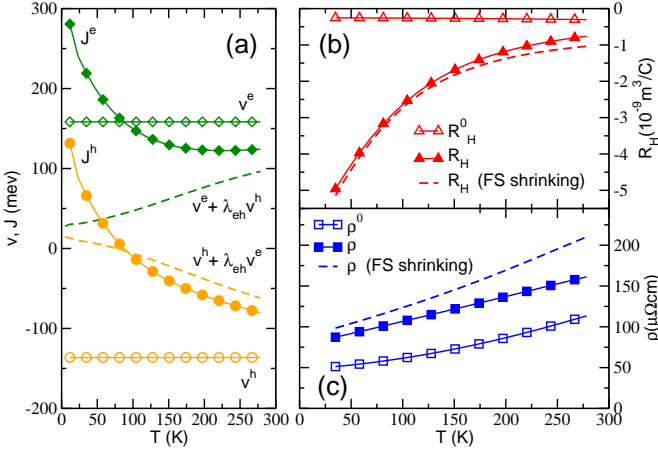


FIG. 1: (a) T dependence of the renormalized currents (filled symbols), as compared to the bare velocities (empty symbols). We also show (dashed lines) the numerators of Eqs. (11)-(12), that fix the overall sign of the currents. (b) T dependence of the Hall coefficient R_H compared to the Boltzmann result (1) R_H^0 , computed with $1/\tau^\alpha = 2\Gamma_F^\alpha$. The units are fixed by the two-dimensional results divided by the interlayer distance $d = 6.5$ Å. Dashed line: R_H obtained including also the effect of the FS shrinking. (c) Longitudinal resistivity as a function of T compared to $\rho^0 = (\sum_\alpha e^2 n_\alpha \tau^\alpha / m)^{-1}$ in the Boltzmann approximation with $1/\tau^\alpha = 2\Gamma_F^\alpha$.

bosonic mode $\chi(\mathbf{q}, i\omega_l)$ of Eq. (7). In Eq. (8) we accounted already for the nesting condition by considering only interband terms, so that the most relevant fluctuations are around $\mathbf{q} = 0$. As far as the vertex corrections are concerned, following a standard derivation[18, 21], the current at $\omega = 0$ is computed as

$$\mathbf{J}^\alpha(\mathbf{k}) = \mathbf{v}^\alpha(\mathbf{k}) + g^2 \sum_{\mathbf{q}} \int_{-\infty}^{\infty} \frac{d\varepsilon}{2\pi} F(\varepsilon) G^{\beta R}(\mathbf{k} + \mathbf{q}, \varepsilon) \times G^{\beta A}(\mathbf{k} + \mathbf{q}, \varepsilon) \text{Im}\chi^R(\mathbf{q}, \varepsilon) \mathbf{J}^\beta(\mathbf{k} + \mathbf{q}). \quad (9)$$

where $F(\varepsilon) = \coth(\varepsilon/2T) - \tanh(\varepsilon/2T)$ and $G^{R,A}$ is the retarded/advanced Green's function. To compute the conductivities (3)-(4) we need the quasiparticle scattering rates Γ_F^α and the dressed currents \mathbf{J}_F^α at the Fermi wavevectors \mathbf{k}_F^α . By accounting for the most relevant contributions to the integrals (8)-(9) one can obtain an approximated semi-analytical expression for all these quantities[28]. The imaginary part of the self-energy is thus given by:

$$\Gamma_F^\alpha = \frac{g^2 \omega_{sf} \chi Q}{2} \sum_{\mathbf{q}} F(\xi_{\mathbf{k}_F^\alpha + \mathbf{q}}^\beta) \frac{\xi_{\mathbf{k}_F^\alpha + \mathbf{q}}^\beta}{\omega_{\mathbf{q}}^2 + (\xi_{\mathbf{k}_F^\alpha + \mathbf{q}}^\beta)^2}, \quad (10)$$

where $\omega_{\mathbf{q}} = \omega_{sf}(1 + \xi_T^2 \mathbf{q}^2)$. At the same time by introducing the velocity and current projection along \mathbf{k} , i.e. $J^\alpha \equiv \mathbf{J}_F^\alpha \cdot \hat{\mathbf{k}}$ and $v^\alpha \equiv \mathbf{v}_F^\alpha \cdot \hat{\mathbf{k}}$, so that $v^h < 0$ and $v^e > 0$, one finds[28] for the renormalized currents the expression

(6) above

$$J^h = (1 - \lambda_{he} \lambda_{eh})^{-1} (v^h + \lambda_{he} v^e) \quad (11)$$

$$J^e = (1 - \lambda_{he} \lambda_{eh})^{-1} (v^e + \lambda_{eh} v^h) \quad (12)$$

where the matrix $\Lambda_{\alpha\beta}$ of Eq. (6) has been expressed in terms of the temperature-dependent coefficients

$$\lambda_{\alpha\beta} = \frac{g^2 \omega_{sf} \chi Q}{2\Gamma_F^\beta} \sum_{\mathbf{q}} F(\xi_{\mathbf{k}_F^\alpha + \mathbf{q}}^\beta) \frac{\xi_{\mathbf{k}_F^\alpha + \mathbf{q}}^\beta}{\omega_{\mathbf{q}}^2 + (\xi_{\mathbf{k}_F^\alpha + \mathbf{q}}^\beta)^2} \frac{\mathbf{k}_F^\alpha + \mathbf{q} \cos \theta_{\mathbf{q}}}{|\mathbf{k}_F^\alpha + \mathbf{q}|}. \quad (13)$$

By close inspection of Eqs.(10) and (13) we see that $\lambda_{\alpha\beta}$ increases as the nesting condition is approached, since the largest contribution to the integrals comes from vectors around $\bar{\mathbf{q}} \sim \mathbf{k}_F^\alpha - \mathbf{k}_F^\beta$. Moreover, at high T where $\xi_T \simeq 0$, so that $\omega_{\mathbf{q}}$ is independent on \mathbf{q} , $\lambda_{\alpha\beta}$ vanishes and $J^\alpha = v^\alpha$. Conversely, at low T , ξ_T increases and only the value $\theta_{\bar{\mathbf{q}}} = 0$ contributes to the integral (13), leading to $\lambda_{\alpha\beta} \rightarrow 1$ and large prefactors in Eqs. (11)-(12).

To elucidate the effect on the transport of such a scattering mechanism connecting e- and h-like bands we will consider a set of parameters appropriate for electron-doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. In particular we take $1/2m = 70$ meV, and we choose $E_{\min}^e = 90$ meV and $E_{\max}^e = 66$ meV (i.e. $k_F^h = 0.30\pi/a$ and $k_F^e = 0.37\pi/a$) to reproduce the data at 7% doping, where long-range AF order is no more present and our model applies. For the SF we use [22] $\omega_0 = 15$ meV, $\Theta = 90$ K, $\xi_0/a = 3.6$ and $g^2 \chi Q = 0.8$ eV. Since the low-energy description (7) is not expected to hold any more around a scale of the order of the room temperature, we rescaled $\xi_T = \xi_0 \sqrt{\Theta/(T + \Theta)} \exp(-T/T_{\text{cut}})$ to account for a fast decay of AF correlations above $T_{\text{cut}} \simeq 300$ K. Finally, to mimic the residual scattering by impurities at $T = 0$ we added a constant (isotropic) scattering rate $\Gamma_0^e = 4$ meV. The resulting currents for each band as a function of temperature, as evaluated from Eqs. (10)-(13), are shown in Fig. 1a, along with the bare Fermi velocities. Two relevant features emerge. First, we find a strong temperature dependence of both J^e and J^h , which deviate significantly from their bare values with lowering temperature, due to the increasing scattering from SF. Second, in the e-doped case considered here, where $|v_e| > |v_h|$, the dominance of $\lambda_{he} v_e$ with respect to v_h in Eq. (11) is reflected in a change of sign of J^h at low T . These features have a striking effect on the Hall transport, shown in Fig. 1b, along with the Boltzmann result (1) computed without vertex corrections. As expected, R_H^0 is small and weakly T dependent, as due to the almost perfect cancellation of the contributions from the h- and e-like Fermi sheets. On the contrary R_H has a strong temperature dependence and it can attain a large negative value at low T , where the e-like renormalized current $|J^e| \gg |J^h|$ dominates the transverse conductivity (4). At the same time, the effects of the vertex renormalization are less qualitatively relevant on the longitudinal resistivity with respect

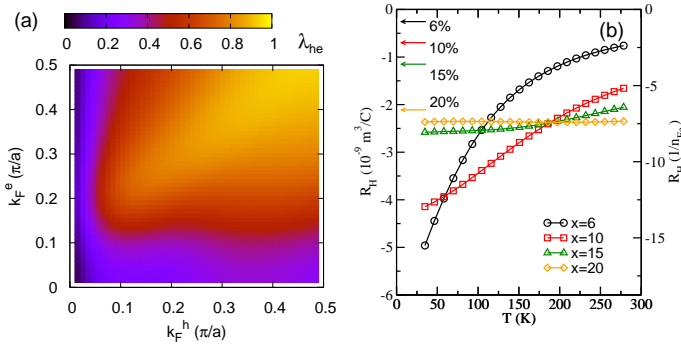


FIG. 2: (Color online) (a) Dependence of the vertex-correction coefficient λ_{he} at $T = 100$ K on the Fermi-wavevectors in the two bands. Notice that λ_{he} decreases as one moves away from the nesting line $k_F^e = k_F^h$. (b) R_H as a function of the Co concentration x (which adds x electrons per Fe atom). The arrows indicate the corresponding values of the $T = 0$ Boltzmann result (1), which has a negligible T dependence on this scale (see Fig. 1b). On the right axes R_H is expressed in units of the inverse number of carriers per Fe atom, defined as $n_{Fe} = 0.32 \times 10^{-9} / |R_H [m^3/C]|$.

to the Boltzmann result, as shown in Fig. 1c. Indeed, the dependence of σ_{xx}^α in Eq. (3) on the sign of the renormalized current leads to a compensation between the vertex corrections in the h and e bands. Our results provide thus a consistent picture for both longitudinal and transverse transport, in good agreement with the experimental findings [3, 4]. For the sake of completeness we show in Fig. 1b,c also the effect of the weakly temperature-dependent FS shrinking arising from the real part of the self-energy (8)[23, 27, 28]. As one can see, this is irrelevant on the Hall transport, while it contributes in part to the temperature dependence of the longitudinal conductivity, as discussed in Ref. [27].

It is also interesting to address the effects of doping. Indeed, as we mentioned above and as we show in Fig. 2a, the absolute value of the $\lambda_{\alpha\beta}$ coefficients decreases as the Fermi wavevectors move away from the nesting condition $k_F^e = k_F^h$, realized at half-filling. We expect thus that the effect of the vertex corrections on the Hall transport will be less relevant by further increasing the Co concentration x . We investigate this issue by making a rigid-band shift of the chemical potential with doping, without changing for simplicity the microscopical parameters of the SF spectrum. The resulting Hall coefficient is reported in Fig. 2b, where we also mark with arrows the corresponding Boltzmann value R_H^0 at each doping. As one can see, the low- T enhancement of R_H induced by SF decreases with increasing doping, and for $x = 20\%$ R_H almost coincides with $R_H^0 \simeq 1/ex$, as found experimentally[3]. The trend shown in Fig. 2b, where SF spectrum is kept constant, is already in good agreement with the experiments.

Nonetheless, one could also expect a decrease of the AF correlation length ξ_T with doping, leading to a faster suppression of vertex corrections. This effect could explain the results in isovalent-substituted systems, as for example $\text{BaFe}_2(\text{As,P/Ru})_2$ [5, 6] or La(Fe,Ru)AsO [7], where the change of magnitude (or even of the sign) of the Hall coefficient should be attributed to a weakening of AF correlations, since no significant change on the FS pockets seems to occur[29]. Finally, we notice that for a hole-doped system the overall temperature and doping dependence of R_H would be exactly the specular one: indeed, when the system is doped with holes, one has in general $k_F^h > k_F^e$, so that $|J^h| \gg |J^e|$ at low T and the transverse conductivity will have a predominant hole-like character, in agreement with the experiments[8, 9]. Thus, the same mechanism accounts for the unusual Hall effect measured in pnictides both in electron and hole-doped compounds.

In conclusion we analyzed the Hall effect in a multi-band model where carriers interact via the exchange of SF. We showed that when interactions have a predominant interband character and connect carriers of opposite e/h nature, the currents renormalized by vertex corrections are dominated by the character of the majority carriers. By evaluating this effect within a simplified two-band model and a phenomenological description of SF we were able to reproduce the main puzzling features observed experimentally in pnictides, namely a strong temperature dependence of R_H with a large absolute value at low T for weak (e or h) doping, and a more ordinary Boltzmann-like behavior at higher doping. We notice that the mechanism discussed here is quite general and robust: thus, an analysis based on a full self-consistent approach for the SF[18] within microscopic multiband models[10, 11] is expected to add only quantitative refinements to the present results. An open question is instead the role of vertex corrections across the antiferromagnetic transition, where the Hall coefficient has been found experimentally to show an even larger T dependence. Even though this issue is beyond the scope of the present manuscript, it certainly deserves further investigation to complete our theoretical understanding of transport properties in pnictides.

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